Phthalic acid, 2,3-dimethylphenyl nonyl ester

Inchi: InChI=1S/C25H32O4/c1-4-5-6-7-8-9-12-18-28-24(26)21-15-10-11-16-22(21)25(27)29-23
InchiKey: BVBQKJNGDFWMNH-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-112.29	kJ/mol	Joback Method
hf	-610.28	kJ/mol	Joback Method
hfus	52.99	kJ/mol	Joback Method
hvap	96.09	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.430		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
tb	992.28	K	Joback Method
tc	1218.63	K	Joback Method
tf	606.23	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.93	J/mol×K	992.28	Joback Method
cpg	1089.16	J/mol×K	1030.01	Joback Method
cpg	1101.89	J/mol×K	1067.73	Joback Method
cpg	1113.19	J/mol×K	1105.46	Joback Method
cpg	1123.09	J/mol×K	1143.18	Joback Method
cpg	1131.64	J/mol×K	1180.91	Joback Method
cpg	1138.88	J/mol×K	1218.63	Joback Method
dvisc	0.0002418	Pa×s	606.23	Joback Method

dvisc	0.0001431	Pa×s	670.57	Joback Method
dvisc	0.0000928	Pa×s	734.91	Joback Method
dvisc	0.0000646	Pa×s	799.25	Joback Method
dvisc	0.0000474	Pa×s	863.60	Joback Method
dvisc	0.0000363	Pa×s	927.94	Joback Method
dvisc	0.0000288	Pa×s	992.28	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume